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General Ray-Tracing Procedure†

G. H. SPENCER* AND M. V. R. K. MURTY
Institute of Optics, University of Rochester, Rochester, New York

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Computing formulas are presented for tracing skew rays through optical systems containing cylindrical and toric surfaces of arbitrary orientation and position. Particular attention is given to the treatment of diffraction gratings and a vector form of the diffraction law is suggested.

INTRODUCTION

ADVANCES in the technology of optical-system fabrication have made practical the design of systems containing nonspherical surfaces. The demands made of modern optical systems, in fact, frequently require the use of unusual surface shapes. Spectrographic and related systems may employ one or more nonspherical gratings, together with refracting or reflecting surfaces in an uncentered configuration.

In order to facilitate the design and analysis of such systems, various techniques of ray tracing have been proposed. Feder[1] has described a computer-oriented procedure for skew-ray tracing through rotationally symmetric systems containing aspheric surfaces. Allen

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[1] D. Feder, J. Opt. Soc. Am. 41, 630 (1951).

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and Snyder[2] have extended Feder's procedure to allow for uncentered configurations of rotationally symmetric surfaces. This procedure requires that the designer specify the direction cosines of the line joining the vertices of adjacent surfaces. Murray[3] has presented a toric skew-ray trace which is suitable for surfaces whose radii are not too large, and Herzberger[4] has given a detailed treatment of quadratic surfaces (conics of revolution, parabolic cylinders, and elliptic paraboloids). More recently, Rosendahl[5] has described a method for ray tracing through systems containing parallel ruled gratings. Yoshinaga, Okazaki, and Tatsuoka[6] also used ray-tracing procedures for evaluating prism and grating spectrometers.

It is the purpose of the present paper to describe a unified ray-tracing procedure applicable to systems of quite general type. The procedure has been developed in accordance with the following requirements:

(1) Cylindrical, toric, and conic surfaces must be accommodated with provision for specifying departures from these forms.

(2) Provision must be made for the arbitrary orientation and positioning of all surfaces with relative ease of specification.

(3) Diffraction gratings generated by linear or concentric circular ruling motions on any of the allowed surface types must be accommodated with provision for specifying a variable ruling separation.

(4) The procedure should be capable of extension to cover new surface types or new modes of ruling without major modification.

In addition, the computing formulas have been tailored for digital-computer use. For this reason, as well as for conceptual simplicity, an algebraic, rather than a trigonometric, approach has been adopted.

DIVISION OF THE PROBLEM

A given ray is specified by the coordinates $(\bar{X}_0,\bar{Y}_0,\bar{Z}_0)$ of a point $\bar{P}_0$ through which the ray passes and by its direction cosines $(\bar{k},\bar{l},\bar{m})$ in a reference coordinate system $(\bar{X},\bar{Y},\bar{Z})$ having its origin at a point $\bar{O}$ (see Fig. 1). A surface S is specified by an equation

$$F(X,Y,Z)=0, \tag{1}$$

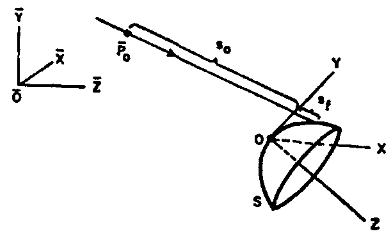

FIG. 1. Reference coordinate system $(\bar{X},\bar{Y},\bar{Z})$ and local system (X,Y,Z), showing incident ray and computed distances, s_0 and s_f.

referred to a coordinate system (X,Y,Z) having its origin at a point O. The orientation of the (X,Y,Z) system relative to the $(\bar{X},\bar{Y},\bar{Z})$ system and the coordinates of O with respect to $\bar{O}$ are given. The ray-tracing problem may now be separated as follows:

(I) Transform the ray-point coordinates $(\bar{X}_0,\bar{Y}_0,\bar{Z}_0)$ and direction cosines $(\bar{k},\bar{l},\bar{m})$ into their values in the (X,Y,Z) system.

(II) Find the point of intersection of the ray with the surface S.

(III) Find the change in direction of the ray refraction, reflection (or diffraction in the case of a grating) at the surface S.

(IV) Transform the new ray-point coordinates and direction cosines back to the $(\bar{X},\bar{Y},\bar{Z})$ system (optional).

(V) Repeat I through IV for succeeding surfaces in sequence.

Step IV is obviously omitted if the coordinate system associated with the next surface is referred to the system associated with S instead of to the reference system.

We now proceed to treat each of the foregoing steps in detail.

I. Transformation to the Local Coordinate System of S

The orientation of the local system (X,Y,Z) may be specified with respect to the reference system in a variety of ways. We have chosen a specification in terms of Euler angles. Figure 2 shows the generation of the (X,Y,Z) system from the $(\bar{X},\bar{Y},\bar{Z})$ system by three successive rotations α, β, and γ. The complete rotation matrix is the product of matrices representing the individual rotations and is

$$\begin{aligned} R &= \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\beta & -\sin\beta \\ 0 & \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\alpha & 0 & -\sin\alpha \\ 0 & 1 & 0 \\ \sin\alpha & 0 & \cos\alpha \end{pmatrix} \\ &= \begin{pmatrix} (\cos\alpha\cos\gamma+\sin\alpha\sin\beta\sin\gamma) & -\cos\beta\sin\gamma & (-\sin\alpha\cos\gamma+\cos\alpha\sin\beta\sin\gamma) \\ (\cos\alpha\sin\gamma-\sin\alpha\sin\beta\cos\gamma) & \cos\beta\cos\gamma & (-\sin\alpha\sin\gamma-\cos\alpha\sin\beta\cos\gamma) \\ \sin\alpha\cos\beta & \sin\beta & \cos\alpha\cos\beta \end{pmatrix}. \end{aligned} \tag{2}$$

All angles shown in Fig. 2 are positive.

[2] W. Allen and J. Snyder, J. Opt. Soc. Am. **42**, 243 (1952).
[3] A. Murray, J. Opt. Soc. Am. **44**, 672 (1954).
[4] M. Herzberger, *Modern Geometrical Optics* (Interscience Publishers, Inc., New York, 1958), Chap. V.
[5] G. Rosendahl, J. Opt. Soc. Am. **51**, 1 (1961).
[6] H. Yoshinaga, B. Okazaki, and S. Tatsuoka, J. Opt. Soc. Am. **50**, 437 (1960).

FIG. 2. Generation of (X,Y,Z) system from $(\bar{X},\bar{Y},\bar{Z})$ system after translation of origin to O. $(\bar{X},\bar{Y},\bar{Z})\rightarrow(\bar{X}',\bar{Y}',\bar{Z}')$ by rotation α; $(X',Y',Z')\rightarrow(X'',Y'',Z'')$ by rotation β; $(X'',Y'',Z'')\rightarrow(X,Y,Z)$ by rotation γ.

The coordinates of the ray point $\bar{P}_0$ in the (X,Y,Z) system will be denoted by (X_0,Y_0,Z_0), and the ray direction cosines in this system will be (k,l,m). If the coordinates of O are $(\bar{x}_0,\bar{y}_0,\bar{z}_0)$, as measured in the reference system, then the transformation equations for the ray data are

$$\begin{bmatrix} X_0 \\ Y_0 \\ Z_0 \end{bmatrix} = R \begin{bmatrix} \bar{X}_0-\bar{x}_0 \\ \bar{Y}_0-\bar{y}_0 \\ \bar{Z}_0-\bar{z}_0 \end{bmatrix}, \tag{3}$$

and

$$\begin{bmatrix} k \\ l \\ m \end{bmatrix} = R \begin{bmatrix} \bar{k} \\ \bar{l} \\ \bar{m} \end{bmatrix}. \tag{4}$$

II. Determination of the Ray Intersection with S

The parametric equations of the given ray may be written

$$X=X_0+ks,\quad Y=Y_0+ls,\quad Z=Z_0+ms, \tag{5}$$

where s is the parameter of distance along the ray measured from (X_0,Y_0,Z_0).

It will be convenient to determine first the intersection of the ray with the $Z=0$ plane. Denoting the required value of s by s_0, and the resulting values of X and Y by X_1 and Y_1, we have from Eqs. (5)

$$s_0=-Z_0/m, \tag{6}$$

$$X_1=X_0+ks_0,\quad Y_1=Y_0+ls_0. \tag{7}$$

With the understanding that s now be measured from $(X_1,Y_1,0)$, we may replace Eqs. (5) by

$$X=X_1+ks,\quad Y=Y_1+ls,\quad Z=ms. \tag{8}$$

Our problem now is to find a value of s such that the resulting values (X,Y,Z) from Eqs. (8) satisfy the surface Eq. (1). We might substitute Eqs. (8) directly in Eq. (1) and attempt to solve the resulting equation for s. This can be accomplished directly, however, only in special cases. Instead, we shall apply the Newton-Raphson iteration technique. Using the subscript j to denote the iteration number, we write,

$$s_{j+1}=s_j-F(X_j,Y_j,Z_j)/F'(X_j,Y_j,Z_j) \tag{9}$$

where from Eqs. (8),

$$X_j=X_1+ks_j,\quad Y_j=Y_1+ls_j,\quad Z_j=ms_j, \tag{10}$$

and where

$$\begin{aligned} F'(X_j,Y_j,Z_j)&=dF/ds_{(s=s_j)} \\ &=(F_x)_jk+(F_y)_jl+(F_z)_jm. \end{aligned} \tag{11}$$

We have used the notation $(F_x)_j$ to represent $\partial F/\partial X$ evaluated at (X_j,Y_j,Z_j), and similarly for the derivatives with respect to Y and Z. The process may be started from a first approximation

$$s_1=0, \tag{12}$$

and is terminated with the value s_f for which

$$|s_f-s_{f-1}|<\epsilon, \tag{13}$$

where ϵ is a small preassigned tolerance whose value depends on the degree of accuracy required.

The choice of a starting point at the $Z=0$ plane will ordinarily ensure convergence of the process represented by Eq. (9) for the forms of the surface equation which we shall define. There are, however, circumstances under which the process will break down or converge to an incorrect value. If $F'\rightarrow 0$ at any point in the process, Eq. (9) will either become indeterminate or will result in $s\rightarrow\infty$. In particular, Eq. (9) will become indeterminate if the ray meets the surface at grazing incidence. It is also possible for $F'\rightarrow 0$ under other circumstances if the surface is nonspherical, but the likelihood of such a situation occurring in practice is fortunately slight. When the ray, in fact, fails to intersect the surface at all, the process will naturally diverge and will usually result in an oscillating sequence of values for s with the possibility of $s\rightarrow\infty$ at some point.

It is further possible for a ray to intersect a surface at several points, and the first approximation (12) may, in such circumstances, result in convergence to an incorrect point. Again, however, the situation is not likely to be encountered in practice.

The total path along the ray from (X_0,Y_0,Z_0) to the surface is

$$p=s_0+s_f. \tag{14}$$

While this quantity is not directly needed for the trace, it provides a quick check on the nature of the ray path. For a true ray path, p must always be positive. A negative value for p indicates a virtual path, i.e., an extension along the line of the ray in the direction opposite to the direction of propagation.

Having completed the iteration, we have the intersection coordinates (X_f,Y_f,Z_f). In addition, we have available a set of direction numbers for the surface normal at the intersection point. These will be needed in step III, and are given by

$$K=(F_x)_f,\quad L=(F_y)_f,\quad M=(F_z)_f. \tag{15}$$

We now turn our attention to the form of the surface equation and its derivatives for various surface types.

TABLE I. Surface obtained for various values of κ.

Range or value of	Type or surface
$\kappa<0$	hyperboloid
$\kappa=0$	paraboloid
$0<\kappa<1$	hemelipsoid of revolution about major axis
$\kappa=1$	hemisphere
$\kappa>1$	hemelipsoid of revolution about minor axis

Rotationally Symmetric Surfaces

All of the rotationally symmetric surfaces encountered in optical design may be represented by

$$F(X,Y,Z)=Z-c\rho^2/[1+(1-\kappa c^2\rho^2)^{\frac{1}{2}}]-\sum_{i=1}^{N}\alpha_i\rho^{2i}=0, \quad (16)$$

where $\rho^2=X^2+Y^2$. In most cases, N need not exceed 5.

If the terms of the summation are omitted, Eq. (16) represents revolved conic sections. The vertex curvature of these surfaces is c, and the type of surface is determined by the value of κ. Table I indicates the type of surface obtained for various values of κ:

Figure 3 clarifies the relationship between c, κ, and the type of surface represented. Note that when $\kappa>0$ the surface Eq. (16) is limited to a range

$$\rho^2<1/(\kappa c^2). \quad (17)$$

The derivatives associated with Eq. (16) are needed, and these are

$$F_x=-XE, \quad F_y=-YE, \quad F_z=1, \quad (18)$$

where

$$E=c/(1-\kappa c^2\rho^2)^{\frac{1}{2}}+2\sum_{j=1}^{N}j\alpha_j\rho^{2(j-1)}. \quad (19)$$

Cones of revolution, or axicons, may be represented by

$$F=Z-\rho/\tan\theta=0, \quad (20)$$

where θ is the half-angle of the cone. The associated derivatives are, then,

$$F_x=-X/\rho\tan\theta, \quad F_y=-Y/\rho\tan\theta, \quad F_z=1. \quad (21)$$

It should be mentioned that Eq. (20) may be closely approximated by the hyperboloid form of Eq. (16) by

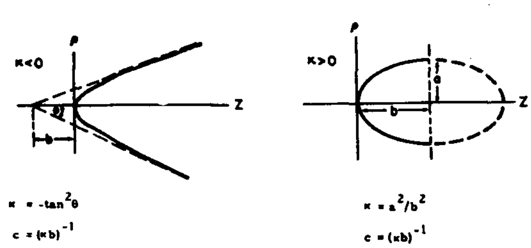

FIG. 3. Relationship of κ and c to geometrical parameters of the conics represented by Eq. (25). The dashed lines in the figure for $\kappa<0$ represent asymptotes.

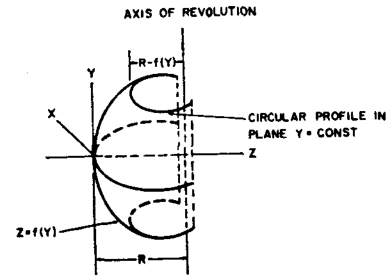

FIG. 4. Generation of toric surface.

giving c a large value and setting

$$\kappa=-\tan^2\theta. \quad (22)$$

The error in this representation satisfies the following conditions:

$$\text{error in } F<|\kappa c|^{-1}, \quad (23)$$

$$\text{error in } dF/d\rho<|2\kappa c^2\rho^2|^{-1}. \quad (24)$$

Finally, it is worthwhile noting that when the terms of the summation in Eq. (16) are omitted, we may avoid taking a square root by writing the surface equation in the simpler form

$$F=Z-\tfrac{1}{2}c(\rho^2+\kappa Z^2)=0. \quad (25)$$

This is essentially the form used by Herzberger[5] in his treatment of conics of revolution. For this case, we have

$$F_x=-cX, \quad F_y=-cY, \quad F_z=1-\kappa cZ. \quad (26)$$

Torics and Cylinders

In the last section, we considered surfaces of revolution about the Z axis. Here, we consider surfaces generated by revolving a curve contained in the YZ plane about an axis parallel to the Y axis, which intersects the Z axis at a distance R from the origin (see Fig. 4). We shall let the equation of the curve in the YZ plane be

$$Z=f(Y). \quad (27)$$

The profile of the surface in a plane parallel to the XZ plane cutting the surface at a height Y will be a circle of radius $R-f(Y)$ with center at $Z=R$, having the equation

$$X^2+(Z-R)^2=[R-f(Y)]^2, \quad (28)$$

or

$$Z=f(Y)+(1/2R)[X^2+Z^2-f^2(Y)]. \quad (29)$$

Defining the curvature of revolution by

$$c_R=1/R, \quad (30)$$

we may thus write

$$F(X,Y,Z)=Z-f(Y)-\tfrac{1}{2}c_R[X^2+Z^2-f^2(Y)]=0, \quad (31)$$

with derivatives

$$F_x=-c_RX,$$
$$F_y=[c_Rf(Y)-1](df/dY), \quad (32)$$
$$F_z=1-c_RZ.$$

We may take a form for $f(Y)$ suggested by Eq. (16):

$$f(Y)=cY^2/[1+(1-\kappa c^2Y^2)^{\frac{1}{2}}]+\sum_{j=1}^{N}\alpha_jY^{2j}. \quad (33)$$

The derivative needed in the second of the Eqs. (32) is thus

$$df/dY=cY/(1-\kappa c^2Y^2)^{\frac{1}{2}}+2\sum_{j=1}^{N}j\alpha_jY^{2(j-1)}. \quad (34)$$

An asphserized cylinder with axis parallel to the X axis is obtained by setting $c_R=0$, while a circular cylinder with axis parallel to the Y axis is obtained by setting $f(Y)=0$.

III. Change in Direction of the Ray after Refraction, Reflection, or Diffraction

Refraction

Snell's law of refraction is most conveniently expressed in the vector form

$$N'\mathbf{S}'\times\mathbf{r}=N\mathbf{S}\times\mathbf{r}. \quad (35)$$

Here $\mathbf{S}$ is a unit vector in the incident-ray direction with components (k,l,m), and $\mathbf{S}'$ is a unit vector in the refracted-ray direction with components (k',l',m'); $\mathbf{r}$ is a vector normal to the refracting surface at the ray intersection point and has components (K,L,M); N is the refractive index of the medium in which the ray is incident and N' is the index of the medium into which the ray is refracted.

It follows from Eq. (35) that

$$\mathbf{S}'=\mu\mathbf{S}+\Gamma\mathbf{r}, \quad (36)$$

where $\mu=N/N'$ and Γ is an undetermined multiplier. The component equations of (36) are

$$k'=\mu k+\Gamma K,\quad l'=\mu l+\Gamma L,\quad m'=\mu m+\Gamma M. \quad (37)$$

Squaring and adding Eqs. (37) we obtain a quadratic in Γ,

$$\Gamma^2+2a\Gamma+b=0, \quad (38)$$

in which

$$a=\mu(kK+lL+mM)/(K^2+L^2+M^2), \quad (39)$$

and

$$b=(\mu^2-1)/(K^2+L^2+M^2). \quad (40)$$

As suggested by Herzberger,[7] Eq. (38) may be solved by the Newton-Raphson iteration technique. We write

$$V(\Gamma)=\Gamma^2+2a\Gamma+b, \quad (41)$$

and use

$$\Gamma_{n+1}=\Gamma_n-V(\Gamma_n)/V'(\Gamma_n). \quad (42)$$

Now,

$$V'(\Gamma_n)=2(\Gamma_n+a),$$

so Eq. (42) becomes

$$\Gamma_{n+1}=(\Gamma_n^2-b)/2(\Gamma_n+a). \quad (43)$$

[7] M. Herzberger, J. Opt. Soc. Am. **41**, 805 (1951).

It is necessary to choose a first approximation Γ_1 which will ensure convergence to the physically correct root of Eq. (38). A suitable value is

$$\Gamma_1=-b/2a. \quad (44)$$

This approximation is seen to break down as $a\rightarrow 0$. However, this corresponds to the case of grazing incidence and, hence, would have resulted in a breakdown in II. The condition under which Eq. (38) fails to have a real root is $b>a^2$, corresponding to total internal reflection.

Reflection

At a reflecting surface we may use the foregoing equations with $\mu=1$ and the other root of Eq. (38). In this case, $b=0$, and we may immediately write

$$\Gamma=-2a. \quad (45)$$

Equations (37) thus become

$$k'=k-2aK,\quad l'=l-2aL,\quad m'=m-2aM. \quad (46)$$

Diffraction

In view of the fact that we have to trace rays in all possible orientations, the usual diffraction equation for the principal section of the grating is inadequate. The general diffraction equations for a plane grating were used in scalar form by, among others, Minkowski[8] in connection with the curvature of spectral lines of grating spectrographs, by Toraldo di Francia[9] in connection with the theory of the Ronchi test, and by Guild[10] in connection with the formation of moiré fringes by two crossed-diffraction gratings. The scalar diffraction equations may be conveniently put in a vectorial form as indicated below.

Consider a plane grating having parallel linear rulings with separation d. Let us associate with the grating a right triple of unit vectors, $\mathbf{p}$, $\mathbf{q}$, and $\mathbf{r}$. Let $\mathbf{r}$ be normal to the grating and $\mathbf{q}$ parallel to the rulings; $\mathbf{p}$ will then be normal to the rulings. Let a beam of light be incident on the grating in a direction defined by the unit vector $\mathbf{S}$. It may be shown that the diffracted beam has a maximum of intensity in the direction of the unit vector $\mathbf{S}'$, satisfying the relation

$$\mathbf{S}'\times\mathbf{r}=\mu\mathbf{S}\times\mathbf{r}+(n\lambda/N'd)\mathbf{q}, \quad (47)$$

where n is the integral order number, λ the vacuum wavelength, and μ and N' are as previously defined. Note that, for the zero order, Eq. (47) becomes Snell's Law.

The following geometrical interpretation of the generalized diffraction relation may be of interest. This is the

[8] R. Minkowski, Astrophys. J. **96**, 305 (1942).

[9] T. di Francia, Contributed article on the Ronchi Test, "Optical image evaluation," NBS Circ. 526, **165** (1954).

[10] J. Guild, *The Interference Systems of Crossed Diffraction Gratings* (Oxford University Press, New York, 1956), p. 23.

fact that all orders of diffraction lie on a cone with ruling direction as the axis and the semi-apex angle equal to the angle made by the zero-order ray with the direction of the rulings.

Now the geometrical-optics approximation allows the laws governing the propagation of a plane wave across an infinite plane boundary to be applied to the propagation of a vanishingly thin pencil of light—the ray—across a local region of a nonplanar boundary. Thus we shall use Eq. (47) as the law determining the direction of the diffracted ray at a point on a grating surface whose shape corresponds to any of the previously given forms of Eq. (1). It will be necessary to determine the local value of d and the local direction of the rulings.

First, let us derive a set of component equations for $\mathbf{S}'$ analogous to Eqs. (37). For convenience, we define

$$\Lambda = n\lambda/N'd. \tag{48}$$

Then, substituting $\mathbf{q} = -\mathbf{p}\times\mathbf{r}$ in Eq. (47), we obtain

$$(\mathbf{S}'-\mu\mathbf{S}+\Lambda\mathbf{p})\times\mathbf{r}=0,$$

from which

$$\mathbf{S}'=\mu\mathbf{S}-\Lambda\mathbf{p}+\Gamma\mathbf{r}. \tag{49}$$

Now, $\mathbf{r}$ need not have unit magnitude in Eq. (49). The value obtained for the multiplier Γ will effectively compensate for a nonunit magnitude of $\mathbf{r}$. Thus, we may take $\mathbf{r}$ to have the components (K,L,M) as determined in II. Denoting the components of $\mathbf{p}$ by (u,v,w) we may write the component equations of (49):

$$\begin{aligned} k'&=\mu k-\Lambda u+\Gamma K,\\ l'&=\mu l-\Lambda v+\Gamma L,\\ m'&=\mu m-\Lambda w+\Gamma M. \end{aligned} \tag{50}$$

Squaring and adding Eqs. (50) and making use of the fact that $\mathbf{p}\cdot\mathbf{r}=0$, we obtain a quadratic equation in Γ:

$$\Gamma^2+2a\Gamma+b'=0, \tag{51}$$

which differs from Eq. (38) only in the value of the last term, given by

$$b'=[\mu^2-1+\Lambda^2-2\mu\Lambda(k\mu+lv+mw)]/(K^2+L^2+M^2). \tag{52}$$

The iteration formula (43) may thus be used to determine Γ:

$$\Gamma_{n+1}=(\Gamma_n{}^2-b')/2(\Gamma_n+a). \tag{53}$$

For a transmission grating, the root of Eq. (51) having the smaller magnitude is required. In this case a suitable first approximation is

$$\Gamma_1=-b'/2a. \tag{54}$$

For the case of a reflection grating, the larger root of Eq. (51) must be taken, and convergence to this root is assured by the first approximation

$$\Gamma_1=b'/2a-2a. \tag{55}$$

The condition under which Eq. (51) fails to have a real root is of the form given in the discussion of refraction: $b'>a^2$.

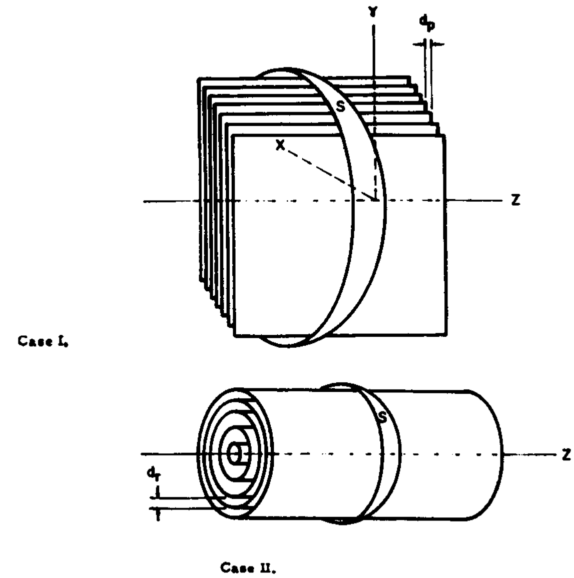

FIG. 5. Mode of grating ruling generation. In Case I, the rulings are defined by the surface intersections with parallel planes. In Case II, the rulings are defined by the intersections with concentric cylinders.

It is now necessary to determine the local grating space d (from which Λ is computed), and the components of $\mathbf{p}$. These quantities depend on the way in which the grating rulings are generated, and we shall consider two cases of interest (see Fig. 5).

Case I. Surface intersections with parallel planes. Here, the grating rulings are defined by the intersections with the surface of a family of parallel planes. The planes are taken to be parallel to the YZ plane and the separation of adjacent planes, d_p, is assumed given by a relation of the form

$$d_p=g(X). \tag{56}$$

In most cases, d_p will be constant, but in special situations it may be desirable to use a variable spacing. In particular, the effects of a periodic ruling error might be studied by including sinusoidal terms in Eq. (56).

Now, $\mathbf{q}$ has no component in the X direction, since it is directed along a grating line which lies in a plane parallel to the YZ plane. Hence,

$$q_x=-(\mathbf{p}\times\mathbf{r})_x=Lw-Mv=0. \tag{57}$$

Also,

$$\mathbf{p}\cdot\mathbf{r}=Ku+Lv+Mw=0, \tag{58}$$

and

$$\mathbf{p}\cdot\mathbf{p}=u^2+v^2+w^2=1. \tag{59}$$

From Eqs. (57)-(59), we obtain

$$\begin{aligned} u&=1/[1+K^2/(L^2+M^2)]^{\frac{1}{2}},\\ v&=-KLu/(L^2+M^2),\\ w&=-KMu/(L^2+M^2). \end{aligned} \tag{60}$$

The local grating space is not given directly by Eq. (56) since the generating planes intersect the surface obliquely. Instead, it is given by $d=d_p/\mathbf{i}\cdot\mathbf{p}$, where $\mathbf{i}$ is the unit normal to the generating planes. Thus,

$$d=d_p/u=g(X)/u. \qquad (61)$$

Case II. Surface intersections with concentric cylinders. In this case, the grating rulings are defined by the intersections with the surface of a family of concentric circular cylinders centered on the Z axis. The radial separation of adjacent cylinders may be taken to be

$$d_r=g(\rho), \qquad (62)$$

where

$$\rho=(X^2+Y^2)^{\frac{1}{2}}.$$

Here, we make use of the fact that ρ is constant along a ruling. This leads to $Xq_x+Yq_y=0$, from which

$$X(Lw-Mv)+Y(Mu-Kw)=0. \qquad (63)$$

Equations (58), (59), and (63) yield

$$\begin{aligned} u&=[M^2X+L(LX-KY)]/G,\\ v&=[M^2Y-K(LX-KY)]/G, \qquad (64)\\ w&=-M(KX+LY)/G, \end{aligned}$$

where

$$G=\{(K^2+L^2+M^2)[M^2\rho^2+(LX-KY)^2]\}^{\frac{1}{2}}. \qquad (65)$$

The local grating space is determined in the same fashion as before:

$$d=d_r/\boldsymbol{\rho}\cdot\mathbf{p},$$

where $\boldsymbol{\rho}$ is the unit normal to the generating cylinders at the point of interest. Thus, we obtain for the grating space

$$d=\rho d_r/(Xu+Yv)=\rho g(\rho)/(Xu+Yv). \qquad (66)$$

IV. Transformation Back to the Reference System

The new ray-point coordinates (X,Y,Z) and direction cosines (k',l',m') may be transformed to the reference system using the inverse forms of Eqs. (3) and (4). Using barred symbols to represent coordinates and cosines in the reference system, we have

$$\begin{pmatrix}\bar{X}\\ \bar{Y}\\ \bar{Z}\end{pmatrix}=R^{-1}\begin{pmatrix}X+\bar{x}_0\\ Y+\bar{y}_0\\ Z+\bar{z}_0\end{pmatrix} \qquad (67)$$

and

$$\begin{pmatrix}\bar{k}'\\ \bar{l}'\\ \bar{m}'\end{pmatrix}=R^{-1}\begin{pmatrix}k'\\ l'\\ m'\end{pmatrix}. \qquad (68)$$

Now, R is a product of unitary matrices and is, therefore, itself unitary. Since a unitary matrix has the property that its inverse equals its transpose, we may write

$$R^{-1}=\begin{pmatrix}(\cos\alpha\cos\gamma+\sin\alpha\sin\beta\sin\gamma) & (\cos\alpha\sin\gamma-\sin\alpha\sin\beta\cos\gamma) & \sin\alpha\cos\beta\\ -\cos\beta\sin\gamma & \cos\beta\cos\gamma & \sin\beta\\ (-\sin\alpha\cos\gamma+\cos\alpha\sin\beta\sin\gamma) & (-\sin\alpha\sin\gamma-\cos\alpha\sin\beta\cos\gamma) & \cos\alpha\cos\beta\end{pmatrix}. \qquad (69)$$

In some situations, particularly when large element separations are involved, it may be desirable from the standpoint of accuracy to retranslate only the X and Y coordinates, setting $\bar{z}_0=0$ in Eq. (67). This establishes a new reference system whose axes are mutually parallel to those of the old system, whose Z axis is collinear with that of the old system, and whose origin is at the point $(0,0,\bar{z}_0)$ as measured in the old system.

In other situations, it may be more convenient to specify the orientation and position of each surface with respect to the local coordinate system of the preceding surface. In these cases, Eqs. (67) and (68) are omitted from the procedure.

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